**United States Environmental Protection Agency** 

Office of Research and Development

### National Exposure Research Laboratory Research Abstract

Government Performance Results Act (GPRA) Goal 1 Annual Performance Measure 236

Significant Research Findings:

## Development of the Unmix Receptor Model for Calculating the Composition and Contributions of Particulate Matter Sources

### Scientific Problem and Policy Issues

Regions of the U.S. that are not in compliance with National Ambient Air Quality Standards (NAAQS) for particulate matter (PM) are required to develop source emissions control strategies. Such strategies depend on estimating the contributions of individual source emissions to PM concentrations in the ambient air in order to better target sources for reduction efforts. The traditional tools for making these estimates have been mathematical air quality simulation models (AQSMs), coupled with emissions inventories and likely meteorological scenarios. Difficulties with this approach include the inability of any AOSM to capture the full complexity of pollutant transport and transformation in the atmosphere, and the uncertainties of emissions rates taken from existing emissions inventories. An alternative to this source-oriented approach is a receptor-oriented one, as embodied in air quality receptor models. Receptor models are mathematical procedures for identifying and quantifying the sources of ambient air pollutants at a site (receptor), primarily on the basis of the concentrations of source-tracing chemical species measured at the receptor and generally without need of emissions inventories and meteorological data. Receptor models are the natural complement to AQSMs, and are used in State Implementation Plans for achieving NAAQS compliance.

### Research Approach

The EPA Unmix receptor model was developed under this project. Unmix is named for its function, which is to "unmix" the concentrations of chemical species measured in the ambient air to identify the contributing sources. The particular mathematical approach used by Unmix is based on a form of Factor Analysis, but its novelty is that physically-meaningful constraints are imposed which are intended to remove the undesirable ambiguity of the multiple solutions that are characteristic of ordinary Factor Analysis. For a given selection of species, Unmix estimates the number of sources, the source compositions, and source contributions to each sample. Chemical profiles of the sources are not required, but instead are generated from the ambient data.

### Results and Impact

The main product of this research is the EPA Unmix 2.3 receptor model. The Unmix model quantifies the sources of particulate matter at a single site using chemical composition data from ambient PM monitoring sites such as the Speciation Trends Network (STN) and Interagency Monitoring for Visual Environments (IMPROVE) sites. The model includes a user-friendly interface for entering input data and selecting variables, as well as for analysis and display of results. EPA Unmix 2.3 is a stand-alone executable program, which requires no

additional software to run.

EPA's Office of Air and Radiation, Office of Transportation and Air Quality, and Regions; State and Local Agencies; and Regional Planning Organizations can use EPA Unmix 2.3 to identify and quantify the sources of PM impacting STN and IMPROVE sites. This information will more effectively guide source control strategies for attaining the PM NAAQS.

### Research Collaboration and Research Products

Collaboration with EPA/NERL on this research effort included contributions from the University of Southern California and from Science Applications International Corporation (SAIC).

The research product is the stand-alone executable version of EPA Unmix 2.3, and it is available on CD.

Examples of recent publications from this study include the following: Lewis, C.W., Norris, G.A., R. C. Henry, R.C., Conner, T.L. "Source Apportionment of Phoenix PM-2.5 Aerosol with the Unmix Receptor Model" *Journal of the Air & Waste Management Association* (2003) 53: 325 - 338.

Mukerjee, S., Norris, G.A., Smith, L.A., Noble, C.A., Neas, L. M, Özkaynak, H.A., Gonzales, M. "Receptor Model Comparisons and Wind Direction Analyses of Volatile Organic Compounds and Submicrometer Particles in an Arid, Binational, Urban Air Shed" *Environmental Science and Technology* (2004) *38*(8) pp 2317 - 2327.

#### **Future Research**

Improvements to EPA Unmix 2.3 are planned to address EPA and external reviewers comments and to increase the functionality of the model. EPA Unmix 2.3 will be modified to report partial results instead of no results when a completely feasible solution cannot be found, report uncertainties of estimated source compositions that account for the effects of serial correlation in the data, apportion total mass and other species not included in model, include an algorithm to replace missing data, and increase speed of finding new solutions and uncertainty calculations.

# Contacts for Additional Information

Questions and inquiries can be directed to the principal investigator:

Gary Norris, Ph.D.
U.S. EPA, Office of Research and Development
National Exposure Research Laboratory
Mail Drop E205-03
109 T.W. Alexander Drive
Research Triangle Park, NC 27711

Phone: 919-541-1519

E-mail: norris.gary@epa.gov

Federal funding for this research was administered under EPA Cooperative Agreement No. CR822072 to the University of Southern California, Contract #s 9D-17226-NATX, 2D-6043-NATX, 3D-6126-NATX, and 3D-6126-NATX to Dr. Ronald Henry; and Contract #68W99002 to Science Applications International Corporation (SAIC).